Published, Nov 23, 2012
Revised, Feb 17, 2014
Revised, March 5, 2020
TFDAO0015.02

Method of Test for Western Medicines as Adulterants in Chinese Medicines and Foods

Preface

This method only lists the common medicines or chemicals which have been ever adulterated. If the suspicious adulteration occurs, it should be investigated.

1. Scope

This method is applicable to the determination of 232 medicines (acetaminophen etc. listed in the attached Table 1) in following samples.

1.1. Traditional or concentrated Chinese medicines, including granule, capsule, oral powder, pillar, tablet, solution, ointment/paste, and patches, and medicinal material and powder.

1.2. Foods, including capsule, tablet, powder and its raw material.

2. Method

After extraction, samples are determined by thin layer chromatography (TLC) and spectrophotometry.

2.1. Equipments

2.1.1. Spectrophotometer.

2.1.2. UV-light coupled with 254 nm and 366 nm.

2.1.3. Ultrasonicator.

2.1.4. Centrifuge.

2.1.5. Rotary evaporator.

2.1.6. Hot plate.

2.1.7. Thermostatic bath.

2.2. Chemicals

Ethanol (95%), *n*-butanol, acetic acid, phosphoric acid, sulfuric acid, hydrochloric acid, ethyl acetate, diethyl ether, chloroform, methanol, ammonia, acetone, bismuth subnitrate, tetrazolium blue, potassium hydroxide, potassium iodide, potassium permanganate, ninhydrin,

p-anisaldehyde, 2,4-dinitrophenylhydrazine, *p*-dimethylaminocinnamaldehyde, *p*-dimethylaminobenzaldehyde, ferric chloride, hydrochloroplatinic acid, mercurous nitrate, vanillin, and iodine, GR grade;
Water, distilled, resistivity ≥ 18 MΩ•cm (at 25°C);
Acetaminophen and other 231 compounds listed in the attached Table 1, reference standards.

2.3. Apparatus

2.3.1. Evaporator flask: 100 mL.

2.3.2. Beaker: 50 mL.

2.3.3. Spray bottle: 50 mL.

2.3.4. Developing tanks: 12 cm × 7 cm × 13 cm, glass.

2.3.5. Centrifuge tube: 15 mL and 50 mL.

2.3.6. TLC plate: silica gel 60 F_{254}, 20 cm × 20 cm (can be customized to 10 cm × 10 cm).

2.3.7. Membrane filter: 0.45 μm, Nylon.

2.3.8. Capillary tube: 5 μL, with scale.

2.4. Developing solvents

2.4.1. *n*-Butanol: water: acetic acid (7:2:1, v/v/v)
Mix *n*-butanol with water and acetic acid at the ratio of 7:2:1 (v/v/v).

2.4.2. Ethyl acetate: diethyl ether (4:1, v/v)
Mix ethyl acetate with diethyl ether at the ratio of 4:1 (v/v).

2.4.3. Chloroform: ethanol (9:1, v/v)
Mix chloroform with ethanol at the ratio of 9:1 (v/v).

2.4.4. Chloroform: ethyl acetate (1:1, v/v)
Mix chloroform with ethyl acetate at the ratio of 1:1 (v/v).

2.4.5. Ethyl acetate: methanol: ammonia (8:1:1, v/v/v)
Mix ethyl acetate with methanol and ammonia at the ratio of 8:1:1 (v/v/v).

2.4.6. Chloroform: diethylamine (2:1, v/v)

Mix chloroform with diethylamine at the ratio of 2:1 (v/v). (only for the identification of betamethasone and dexamethasone)

2.5. Reagents

2.5.1. 6 N potassium hydroxide

Dissolve 33.7 g of potassium hydroxide with water to 100 mL.

2.5.2. 6 N hydrochloric acid

Dissolve 49.4 mL of hydrochloric acid with water to 100 mL.

2.6. Spray reagents

2.6.1. Dragendorff's reagent

2.6.1.1. Solution A: Dissolve 2 g of bismuth nitrate with 25 mL of acetic acid and 100 mL of water, and then store in a refrigerator.

2.6.1.2. Solution B: Dissolve 40 g of potassium iodide with 100 mL of water, and then store in a refrigerator.

2.6.1.3. When to use, mix equal volume of solution A and B.

2.6.2. 50% sulfuric acid in ethanol(note)

Mix equal volume of sulfuric acid and 95% ethanol.

2.6.3. Iodine vapor

Weigh appropriate amount of iodine, and place in a closed container.

2.6.4. Tetrazolium blue reagent

Dissolve 0.5 g of tetrazolium blue with 100 mL of methanol, and then store in a refrigerator. When to use, mix with equal volume of 6 N potassium hydroxide.

2.6.5. *p*-Dimethylaminobenzaldehyde reagent(note)

Dissolve 2 g of *p*-dimethylaminobenzaldehyde with 2 mL of water and 18 mL of sulfuric acid, and cool down.

2.6.6. Ninhydrin reagent(note)

Dissolve 0.1 g of ninhydrin with 20 mL of acetone.

2.6.7. *p*-Anisaldehyde reagent(note)

Dissolve 0.5 mL of *p*-anisaldehyde reagent with 0.1 mL of acetic acid, 0.5 mL of sulfuric acid and 9 mL of ethanol.

2.6.8. 2,4-Dinitrophenylhydrazine reagent

Dissolve 0.3 g of 2,4-dinitrophenylhydrazine with 20 mL of sulfuric acid : water (1:1, v/v).

2.6.9. *p*-Dimethylaminocinnamaldehyde reagent

Dissolve 2 g of *p*-dimethylaminocinnamaldehyde with 100 mL of 6 N hydrochloric acid and 100 mL of ethanol. When to use, mix with four times volume of ethanol.

2.6.10. 5% ferric chloride reagent

Dissolve 1 g of ferric chloride with 20 mL of water.

2.6.11. Iodoplatinate reagent

Dissolve 0.04 g of potassium chloroplatinate and 1 g of potassium iodide with 20 mL of water.

2.6.12. Acidified iodoplatinate reagent

Mix 20 mL of iodoplatinate reagent with 0.4 mL of HCl. The reagent should be used within 2 weeks after preparation.

2.6.13. 1% mercurous nitrate

Dissolve 0.2 g of mercurous nitrate with 20 mL of water.

2.6.14. 1% potassium permanganate

Dissolve 0.2 g of potassium permanganate with 20 mL of water.

2.6.15. 1% vanillin(note)

Dissolve 0.2 g of vanillin with 20 mL of sulfuric acid.

Note：After spraying the TLC plate with the reagent, heat the plate on a hot plate until the spots appear.

2.7. Standard solution preparation

Accurately weigh equivalent 10 mg of reference standards to each 10-mL volumetric flask, dissolve and dilute with ethanol to volume as standard solutions.

2.8. Sample solution preparation

2.8.1. Granule, oral powder, powder and medicinal powder

Transfer about 5 g of a well-mixed sample into a 50-mL centrifuge tube, dilute with appropriate amount of ethanol (about 3~4 times volume of sample weight depending on the property of the sample), and ultrasonicate for 30 min. After standing, filter the supernatant with a membrane filter and take the filtrate as the sample solution.

2.8.2. Capsule

Use about 5 g of the sample and pour out its contents. Transfer both contents and capsule shells into a 50-mL centrifuge tube, dilute with appropriate amount of ethanol (about 3~4 times volume of sample weight depending on the property of the sample), and ultrasonicate for 30 min. After standing, filter the supernatant with a membrane filter and take the filtrate as the sample solution.

2.8.3. Tablet, pillar, patches and medicinal material

After grinding or cutting, transfer about 5 g of the sample into a 50-mL centrifuge tube, dilute with appropriate amount of ethanol (about 3~4 times volume of sample weight depending on the property of the sample), and ultrasonicate for 30 min. After standing, filter the supernatant with a membrane filter and take the filtrate as the sample solution.

2.8.4. Solution

Transfer about 40 mL of the sample into a evaporator flask, and concentrate to dryness under reduced pressure at 40^{o}C. Add 10 mL of ethanol, and ultrasonicate for 30 min. After standing, filter the supernatant with a membrane filter and take the filtrate as the sample solution.

2.8.5. Ointment/paste

Transfer about 5 g of the sample into a beaker, dissolve with 20 mL of ethanol in a water bath at 40^{o}C and mix well. After standing at 0^{o}C for 2 hrs, filter the supernatant

with a membrane filter and take the filtrate as the sample solution.

2.9. Identification

2.9.1. Prepare 4 developing solvents according to section 2.4.1.-2.4.5., in which choose either ethyl acetate: diethyl ether (4:1, v/v) or chloroform: ethyl acetate (1:1, v/v), and transfer appropriate amount of the developing solvents into TLC developing tanks, and stand for 5 min to achieve saturation.

2.9.2. Use capillary tubes to apply the sample and the standard solutions on a TLC plate (10 × 10 cm). The band length of the sample solution is about 1 to 2 cm, and the band length of the standard solutions are about 0.5 cm. Label the marks represent the sample, standard, and the developing solvent on the TLC plate. Observe the darkness of the sample spot under UV light to adjust the suitable applying number.

2.9.3. Place the TLC plates into the TLC developing tanks for development.

2.9.4. After air-drying, observe the TLC plates under a UV lamp with the wavelength of 254 or 366 nm, and mark the suspected spot by a pencil.

2.9.5. Scrap the suspected spot and transfer into a centrifuge tube. Add 3 mL of ethanol and ultrasonicate for 5 min. Centrifuge at 3000 rpm for 10 min, and determine the supernatant by the spectrophotometer. Compare the UV absorption spectrum of the sample with those of reference standards for identification.

2.9.6. If there are suspected drugs in the sample, identified by the UV absorption spectrum, repeat the procedure in section 2.9.1.~2.9.5. Use the targeted reference standard for confirmation according to the R_f value with the same mobile phase. (R_f value is defined as the ratio

of the distance moved by the sample spot to the distance moved by the solvent.)

2.9.7. Choose the spray reagent according to the targeted compounds listed in the attached Table 2, spray it on the TLC plate, and record the color of spot.

2.10. Decision making

The UV absorption spectrum, R_f value and color reaction of the sample spot on the TLC plate are consistent with those of the reference standard as a positive result, otherwise as a negative result.

Remark

1. TLC is suitable to monitor the compounds which may have UV-absorption, or have the coloring reaction with spray reagents. The complicated matrix in Chinese medicines or foods may interfere with the reaction and result. Further validation shall be done when interference compounds appear in samples, such as modifying the developing solvent or spray reagent.
2. If the targeted compound has been detected by this method, the GC-MS or LC-MS/MS method should be used to confirm the results. The parameters of analytes by GC-MS and LC-MS/MS are listed in the attached Table 3 and Table 4, respectively.
3. When use the TLC scanner instead of the spectrophotometer, the method should be validated.

Published, Nov 23, 2012
Revised, Feb 17, 2014
Revised, March 5, 2020
TFDAO0015.02

Table 1. The categories and compounds of medicines adulterated in Chinese medicines or foods

Category	Compound
Tonify the kidney (Erectile dysfunction treatment)	Acetil acid, Acetildenafil, Acetylvardenafil, Aminotadalafil, Avanafil, Caffeine, Carbodenafil, Chloropretadalafil, *N*-Desethylacetildenafil, *N*-Desethylvardenafil, *N*-Desmethylsildenafil, Desulfovardenafil, Dimethylsildenafil, Fluoxymesterone, Gendenafil, Homosildenafil, Hydroxyacetildenafil, Hydroxyhomosildenafil, Hydroxythiohomosildenafil, Hydroxyvardenafil, Imidazosagatriazinone, 7-Ketodehydroepiandrosterone, Methyltestosterone, Noracetildenafil, Norneosildenafil, Nortadalafil, Phentolamine, Piperiacetildenafil, Piperidenafil, Sildenafil, Tadalafil, Testosterone, Thiodimethylsildenafil, Thiohomosildenafil, Thiosildenafil, Vardenafil, Yohimbine
Weight loss	Caffeine, Cetilistat, Clobenzorex, Desacetyl bisacodyl, *N*-Desmethylsibutramine, *N*-Didesmethylsibutramine, Diethylpropion, 2-Diphenylmethylpyrrolidine (Desoxy-D2PM), Fenfluramine, Fluoxetine, Lorcaserin, Mazindol, Mephentermine, Methamphetamine, Orlistat, Phenolphthalein, Phentermine, Phenylpropanolamine, Rimonabant, Sibutramine, Synephrine
Cold preparation	Acetaminophen, Aminopyrine, Aspirin, Benproperine, Bromhexine, Bucetin, Caffeine, Carbetapentane, Carbinoxamine, Chlorpheniramine, Cyproheptadine, Dextromethorphan, Diprophylline, Ethoxybenzamide, Guaifenesin, Phenacetin, Phenylephrine, Promethazine, Terfenadine
Steroids	Betamethasone, Cortisone, Dexamethasone, Hydrocortisone, Methylprednisolone, Prednisolone, Prednisone, Triamcinolone
Relieve rheumatism and pain	Acetaminophen, Aminopyrine, Aspirin, Bucetin, Carisoprodol, Celecoxib, Chlormezanone, Chlorzoxazone, Dexamethasone, Diclofenac, Ethoxybenzamide, Ibuprofen, Indomethacin, Ketoprofen, Mefenamic acid, Naproxen, Nefopam, Oxyphenbutazone, Phenylbutazone, Piroxicam, Prednisolone, Salicylamide, Sulindac
Painkiller	Acetaminophen, Aminopyrine, Aspirin, Bucetin, Celecoxib, Ethoxybenzamide, Ibuprofen, Mefenamic acid, Nefopam, Piroxicam, Salicylamide, Sulindac
Traumatic injuries treatment	Acetaminophen, Guaifenesin, Indomethacin, Phenacetin, Phenylbutazone
Antiasthmatic	Chlorpheniramine, Dexamethasone, Dextromethorphan, Diprophylline, Prednisolone, Theophylline
Aphrodisiac	Amphetamine, Methamphetamine, Methyltestosterone, Morphine, Pentazocine, Strychnine, Testosterone, Yohimbine
Topical anesthesia	Benzocaine, Cocaine, Dibucaine, Lidocaine, Prilocaine, Procaine, Testosterone, Tetracaine, Yohimbine
Invigorating the stomach function	Atropine, Butropium, Camylofine, Cimetidine, Dicyclomine, Famotidine, Glycopyrronium, Homatropine, Metoclopramide, Omeprazole, Oxethazaine, Oxyphencyclimine, Pirenzepine, Propantheline, Ranitidine, Scopolamine

Category	Compound
Anticonvulsants for infant	Acetaminophen, Aminopyrine, Aspirin, Chlordiazepoxide, Diazepam, Phenacetin, Quinine
Detoxification	Chloramphenicol, Sulfadiazine, Sulfadimethoxine, Sulfamerazine, Sulfamethazine, Sulfamethoxazole, Sulfamethoxypyridazine, Sulfanilamide, Sulfathiazole, Sulfisoxazole
Laxatives	Bisacodyl
Antidiabetic	Acetohexamide, Chlorpropamide, Glibenclamide, Metformin, Phenformin, Pioglitazone, Rosiglitazone, Tolbutamide
Treatment of arteriosclerosis, vasodilator	Bezafibrate, Clofibrate, Etofibrate, Fenofibrate, Gemfibrozil, Nicametate, Nylidrin, Xanthinol Niacinate
Antiallergic	Brompheniramine, Carbinoxamine, Chlorpheniramine, Cyproheptadine, Diphenhydramine, Hydroxyzine, Terfenadine
Sedative	Amitriptyline, Barbital, Bromvalerylurea, Chlordiazepoxide, Chlorpromazine, Clozapine, Diazepam, Fluoxetine, Lorazepam, Melatonin, Meprobamate, Methaqualone, Phenobarbital, Secobarbital, Thioridazine, Zolpidem
Antihypertensive, diuretic	Chlorothiazide, Cinnarizine, Dipyridamole, Furosemide, Hydralazine, Hydrochlorothiazide, Propranolol, Reserpine, Spironolactone
Regulating menstruation and vaginitis treatment	Estradiol, Ethinylestradiol, Metronidazole, Progesterone, Tinidazole
Estrogen-like	Diethylstilbestrol, Estradiol, Estriol, Estrone,Ethinylestradiol, Ethisterone, Norethisterone, Norgestrel, Progesterone
Urinary system ailments treatment	Flavoxate, Nalidixic acid, Nitrofurantoin, Norfloxacin, Phenazopyridine, Sulfamethizole, Sulfisoxazole, Trimethoprim
Anabolic hormones	Ethylestrenol, Methandriol, Methandrostenolone, Nandrolone, Oxymetholone, Stanozolol
Antiepileptic, anticonvulants	Benzhexol, Diphenylhydantoin, Mephenesin, Metharbital, Orphenadrine, Phenobarbital, Primidone, Topiramate
Cardiotonic agent	Caffeine, Digitoxin
Cardiac agents	Atenolol, Dipyridamole, Nifedipine, Propranolol
Uricosuric agents and antigout	Allopurinol, Benzbromarone, Colchicine, Probenecid, Sulfinpyrazone
Thyroid disorder Treatment	Carbimazole, Liothyronine, Methimazole
Eye protection	Cortisone, Diclofenac, Sulfamethoxazole
Psychostimulant	Atropine, Caffeine, Pentazocine, Strychnine, Theobromine
Antifungal	Econazole, Ketoconazole, Terbinafine
Baldness treatment	Estriol, Finasteride, Griseofulvin, Ketoconazole, Minoxidil, Prednisolone, Salicylic acid

Category	Compound
Topical ointment, powder	Chlorpheniramine, Cortisone, Dexamethasone, Diphenhydramine, Prednisolone, Salicylic acid

Published, Nov 23, 2012
Revised, Feb 17, 2014
Revised, March 5, 2020
TFDAO0015.02

Table 2. The recommended spray reagents on each category of medicines adulterated in Chinese medicines or foods

Category	Spray reagent (recommend)
Tonify the kidney (Erectile dysfunction treatment)	Dragendorff's reagent; 50% sulfuric acid ethanol solvent; Acidification of iodoplatinate solution
Weight loss	Dragendorff's reagent; 50% sulfuric acid ethanol solvent; Ninhydrin solution
Cold preparation	Dragendorff's reagent; 50% sulfuric acid ethanol solvent; Iodine vapor; Ninhydrin solution; 1% potassium permanganate solution; 1% vanillin solution
Steroids	Dragendorff's reagent; 50% sulfuric acid ethanol solvent; tetrazolium blue solution; 1% vanillin solution
Relieve rheumatism and pain	Dragendorff's reagent; 50% sulfuric acid ethanol solvent; Iodine vapor; 2,4-dinitrophenylhydrazine solution; 5% ferric chloride solution; 1% vanillin solution
Painkiller	Dragendorff's reagent; 50% sulfuric acid ethanol solvent; Iodine vapor; *p*-Anisaldehyde solution; 5% ferric chloride solution
Traumatic injuries treatment	Dragendorff's reagent; 50% sulfuric acid ethanol solvent; Iodine vapor
Antiasthmatic	Dragendorff's reagent; 50% sulfuric acid ethanol solvent; Iodine vapor; Ninhydrin solution; 1% potassium permanganate solution
Aphrodisiac	Dragendorff's reagent; 50% sulfuric acid ethanol solvent; Iodine vapor; Acidification of iodoplatinate solution; 1% potassium permanganate solution
Topical anesthesia	Dragendorff's reagent; Iodine vapor; Acidification of iodoplatinate solution; Ninhydrin solution
Invigorating the stomach function	Dragendorff's reagent; 50% sulfuric acid ethanol solvent; *p*-Anisaldehyde solution
Anticonvulsants for infant	Dragendorff's reagent; 50% sulfuric acid ethanol solvent; *p*-Dimethylaminobenzaldehyde solution; *p*-Dimethylaminocinnamaldehyde solution
Detoxification	*p*-Dimethylaminobenzaldehyde solution; *p*-Dimethylaminocinnamaldehyde solution; 1% vanillin solution
Laxatives	Dragendorff's reagent
Antidiabetic	Dragendorff's reagent; Ninhydrin solution; 1% vanillin solution
Treatment of arteriosclerosis, vasodilator	Dragendorff's reagent; 50% sulfuric acid ethanol solvent; Iodine vapor; Acidification of iodoplatinate solution; 1% potassium permanganate solution
Antiallergic	Iodine vapor; Iodoplatinate solution; Acidification of Iodoplatinate solution
Sedative	Dragendorff's reagent; Iodine vapor; *p*-Anisaldehyde solution; 1% mercurous nitrate solution

Category	Spray reagent (recommend)
Antihypertensive, diuretic	Dragendorff's reagent; Iodine vapor; Acidification of iodoplatinate solution; 1% potassium permanganate solution; 1% vanillin solution
Regulating menstruation and vaginitis treatment	50% sulfuric acid ethanol solvent
Estrogen-like	50% sulfuric acid ethanol solvent
Urinary system ailments treatment	Dragendorff's reagent; Iodine vapor; *p*-Dimethylaminobenzaldehyde solution*; p*-Dimethylaminocinnamaldehyde solution
Anabolic hormones	50% sulfuric acid ethanol solvent
Antiepileptic, anticonvulants	Iodine vapor; Iodoplatinate solution; 1% mercurous nitrate solution; 1% potassium permanganate solution
Cardiotonic agent	Dragendorff's reagent; 50% sulfuric acid ethanol solvent
Cardiac agents	Dragendorff's reagent; Iodoplatinate solution; Acidification of iodoplatinate solution
Uricosuric agents and antigout	Dragendorff's reagent; *p*-Anisaldehyde solution; 1% potassium permanganate solution
Thyroid disorder Treatment	Dragendorff's reagent; Iodine vapor
Eye protection	*p*-Dimethylaminobenzaldehyde solution; *p*-Dimethylaminocinnamaldehyde solution
Psychostimulant	Dragendorff's reagent; 50% sulfuric acid ethanol solvent; Iodine vapor; Acidification of iodoplatinate solution
Antifungal	Dragendorff's reagent; 50% sulfuric acid ethanol solvent; Ninhydrin solution
Baldness treatment	Dragendorff's reagent; 50% sulfuric acid ethanol solvent; 5% ferric chloride solution
Topical ointment, powder	Dragendorff's reagent; 50% sulfuric acid ethanol solvent; Iodine vapor; 5% ferric chloride solution

Note: If the adulteration occurred but out of above categories of medicines, the spray reagent should be chosen according to the chemical property of the suspected medicine.

Published, Nov 23, 2012
Revised, Feb 17, 2014
Revised, March 5, 2020
TFDAO0015.02

Table 3. The parameters of 232 medicines analyzed by GC-MS

NO.	Compound	Molecular formula	Molecular weight	Qualitation ion (*m/z*)
1	Acetaminophen	$C_8H_9NO_2$	151	151, 109, 80, 83
2	Acetil acid	$C_{18}H_{20}N_4O_4$	356	—
3	Acetildenafil	$C_{25}H_{34}N_6O_3$	466	127, 70, 84, 42, 112, 56, 98
4	Acetohexamide	$C_{15}H_{20}N_2O_4S$	324	199, 184, 120, 104, 91, 76, 64, 51
5	Acetylvardenafil	$C_{25}H_{34}N_6O_3$	466	—
6	Allopurinol	$C_5H_4N_4O$	136	136, 52, 109, 120, 67
7	Aminopyrine	$C_{13}H_{17}N_3O$	231	231, 97, 77, 56
8	Aminotadalafil	$C_{21}H_{18}N_4O_4$	390	390, 262, 204, 289, 233, 102, 169, 375, 43, 405
9	Amitriptyline	$C_{20}H_{23}N$	277	277, 202, 178, 152, 115, 91, 58
10	Amphetamine	$C_9H_{13}N$	135	44, 91,65,120
11	Aspirin	$C_9H_8O_4$	180	120, 92, 152, 65, 45
12	Atenolol	$C_{14}H_{22}N_2O_3$	266	222, 107, 72
13	Atropine	$C_{17}H_{23}NO_3$	289	124, 82, 94, 289, 140, 67, 103, 42
14	Barbital	$C_8H_{12}N_2O_3$	184	156, 141, 98, 112, 55, 41, 83, 69
15	Benzbromarone	$C_{17}H_{12}Br_2O_3$	424	264, 173, 279, 115, 249, 328, 145, 132, 221
16	Benzhexol	$C_{20}H_{31}NO$	301	—
17	Benzocaine	$C_9H_{11}NO_2$	165	165, 120, 92, 65
18	Betamethasone	$C_{22}H_{29}FO_5$	392	312, 281, 207, 160, 122, 91, 55
19	Bezafibrate	$C_{19}H_{20}ClNO_4$	361	120, 139, 107, 77, 156
20	Bisacodyl	$C_{22}H_{19}NO_4$	361	361, 319, 276, 246, 199, 154
21	Bromhexine	$C_{14}H_{20}Br_2N_2$	376	376, 293, 264, 112, 70, 374
22	Brompheniramine	$C_{16}H_{19}BrN_2$	318	247, 58, 167, 72, 180, 42, 139
23	Bromvalerylurea	$C_6H_{11}BrN_2O_2$	222	137, 44, 100, 55, 83, 69, 120
24	Bucetin	$C_{12}H_{17}NO_3$	223	223, 137, 108, 81, 53
25	Butropium	$C_{28}H_{38}NO_4^+$	452	—
26	Caffeine	$C_8H_{10}N_4O_2$	194	194, 109, 67
27	Camylofine	$C_{19}H_{32}N_2O_2$	320	—
28	Carbetapentane	$C_{20}H_{31}NO_3$	333	86, 144, 115, 100, 58, 100, 115
29	Carbimazole	$C_7H_{10}N_2O_2S$	186	186, 114, 72, 81, 42, 56, 127, 141
30	Carbinoxamine	$C_{16}H_{19}ClN_2O$	290	201, 167, 139, 71
31	Carbodenafil	$C_{24}H_{32}O_3N_6$	452	84, 56, 70, 381, 452, 339, 311, 42, 113, 136
32	Carisoprodol	$C_{12}H_{24}N_2O_4$	260	245, 184, 158, 97, 83, 69, 55

NO.	Compound	Molecular formula	Molecular weight	Qualitation ion (*m/z*)
33	Chloramphenicol	$C_{11}H_{12}Cl_2N_2O_5$	322	207, 172,153, 106, 77
34	Chlordiazepoxide	$C_{16}H_{14}ClN_3O$	299	282, 247, 220, 190, 165, 124, 91
35	Chlormezanone	$C_{11}H_{12}ClNO_3S$	273	208, 174, 152, 125, 98, 69
36	Chloropretadalafil	$C_{22}H_{19}ClN_2O_5$	426	—
37	Chlorothiazide	$C_7H_6ClN_3O_4S_2$	295	—
38	Chlorpheniramine	$C_{16}H_{19}ClN_2$	274	203, 58, 167, 72, 180, 42
39	Chlorpromazine	$C_{17}H_{19}ClN_2S$	318	318, 272, 232, 196, 86, 58
40	Chlorpropamide	$C_{10}H_{13}ClN_2O_3S$	276	190, 174, 127, 111, 75
41	Chlorzoxazone	$C_7H_4ClNO_2$	169	169, 113, 78
42	Cimetidine	$C_{10}H_{16}N_6S$	252	45, 116, 55, 70, 60, 74, 42, 88
43	Cinnarizine	$C_{26}H_{28}N_2$	368	201, 117, 167, 251, 152, 91
44	Clobenzorex	$C_{16}H_{18}ClN$	259	168, 127, 91, 65
45	Clofibrate	$C_{12}H_{15}ClO_3$	242	242, 169, 128
46	Cocaine	$C_{17}H_{21}NO_4$	303	182, 82, 303, 105, 272, 198, 122, 51
47	Colchicine	$C_{22}H_{25}NO_6$	399	399, 371, 312, 281, 254
48	Cortisone	$C_{21}H_{28}O_5$	360	122, 300, 91, 256, 105, 77, 147, 161, 55
49	7-keto-Dehydroepiandroster-one (7-keto-DHEA)	$C_{19}H_{26}O_3$	302	302, 161, 91, 79, 105, 134, 187, 55, 41, 205
50	*N*-Desethylvardenafil	$C_{21}H_{28}N_6O_4S$	460	—
51	*N*-Desethylacetildenafil	$C_{23}H_{30}N_6O_3$	438	—
52	*N*-Desmethylsibutramine	$C_{16}H_{24}ClN$	265	100, 58, 44, 137, 128, 115
53	*N*-Desmethylsildenafil	$C_{21}H_{28}N_6O_4S$	460	—
54	*N*-Didesmethylsibutramine	$C_{15}H_{22}ClN$	251	137, 115, 86
55	Dexamethasone	$C_{22}H_{29}FO_5$	392	312, 160, 122, 91, 55
56	Dextromethorphan	$C_{18}H_{25}NO$	271	271, 150, 214, 59, 171, 203, 128
57	Diazepam	$C_{16}H_{13}ClN_2O$	284	283, 256, 221, 165, 77, 51
58	Dibucaine	$C_{20}H_{29}N_3O_2$	343	116, 86, 58
59	Diclofenac	$C_{14}H_{11}Cl_2NO_2$	295	295, 242, 214, 179, 151
60	Dicyclomine	$C_{19}H_{35}NO_2$	309	86, 55
61	Diethylpropion	$C_{13}H_{19}NO$	205	100, 77, 51
62	Diethylstilbestrol	$C_{18}H_{20}O_2$	268	268, 239, 145, 107
63	Digitoxin	$C_{41}H_{64}O_{13}$	764	—
64	Dimethylsildenafil	$C_{23}H_{32}O_4N_6S$	488	113, 312, 70, 84, 42, 283, 136
65	Diphenhydramine	$C_{17}H_{21}NO$	255	165, 58
66	Diphenylhydantoin	$C_{15}H_{12}N_2O_2$	252	180, 223, 209, 252, 104, 77, 165, 147, 51
67	Diprophylline	$C_{10}H_{14}N_4O_4$	254	254, 223, 180, 137, 109, 81, 54

NO.	Compound	Molecular formula	Molecular weight	Qualitation ion (*m/z*)
68	Dipyridamole	$C_{24}H_{40}N_8O_4$	504	—
69	Econazole	$C_{18}H_{15}Cl_3N_2O$	380	299, 207, 125, 81, 54
70	Estradiol	$C_{18}H_{24}O_2$	272	272, 146, 160, 145, 159, 213, 172
71	Estriol	$C_{18}H_{24}O_3$	288	288, 160, 146, 213, 133, 172, 201, 115, 185
72	Estrone	$C_{18}H_{22}O_2$	270	270, 146, 285, 213
73	Ethinylestradiol	$C_{20}H_{24}O_2$	296	213, 296, 160, 133, 145, 228, 172, 185, 115
74	Ethisterone	$C_{21}H_{28}O_2$	312	124, 312, 91, 229, 245, 79, 105, 148, 286, 189, 67
75	Ethoxybenzamide	$C_9H_{11}NO_2$	165	165, 150, 120, 92, 65
76	Ethylestrenol	$C_{20}H_{32}O$	288	216, 241, 201, 288, 91, 270, 79, 121, 147, 105
77	Etofibrate	$C_{18}H_{18}ClNO_5$	363	—
78	Fenfluramine	$C_{12}H_{16}F_3N$	231	159, 109, 72, 56
79	Fenofibrate	$C_{20}H_{21}ClO_4$	360	—
80	Finasteride (Proscar)	$C_{23}H_{36}N_2O_2$	372	372, 110, 58, 272, 357, 258, 128, 230, 72, 245
81	Flavoxate	$C_{24}H_{25}NO_4$	391	263, 234, 147, 98
82	Fluoxetine	$C_{17}H_{18}F_3NO$	309	309, 183, 162, 133, 104, 78, 59
83	Fluoxymesterone	$C_{20}H_{29}FO_3$	336	336, 279, 109, 71
84	Furosemide	$C_{12}H_{11}ClN_2O_5S$	330	—
85	Gemfibrozil	$C_{15}H_{22}O_3$	250	250, 122
86	Gendenafil	$C_{19}H_{22}N_4O_3$	354	354, 326, 339, 136, 166, 282, 43, 311, 297
87	Glibenclamide	$C_{23}H_{28}ClN_3O_5S$	493	—
88	Glycopyrronium	$C_{19}H_{28}NO_3^+$	317	—
89	Griseofulvin	$C_{17}H_{17}ClO_6$	352	352, 310, 284, 254, 214, 171, 138, 95, 69
90	Guaifenesin	$C_{10}H_{14}O_4$	198	124, 109,198,77,95,65,52,167,149
91	Homatropine	$C_{16}H_{21}NO_3$	275	275, 124, 79
92	Homosildenafil	$C_{23}H_{32}N_6O_4S$	488	113, 70, 281, 56, 42, 207, 355, 341, 309, 253
93	Hydralazine	$C_8H_8N_4$	160	160, 103, 131, 115, 89, 76, 145, 63, 50
94	Hydrochlorothiazide	$C_7H_8ClN_3O_4S_2$	297	—
95	Hydrocortisone	$C_{21}H_{30}O_5$	362	305, 163, 123, 91, 55
96	Hydroxyacetildenafil	$C_{25}H_{34}N_6O_4$	482	—
97	Hydroxyhomosildenafil	$C_{23}H_{32}N_6O_5S$	504	—
98	Hydroxythiohomosildenafil	$C_{23}H_{32}N_6O_4S_2$	520	—

Published, Nov 23, 2012
Revised, Feb 17, 2014
Revised, March 5, 2020
TFDAO0015.02

NO.	Compound	Molecular formula	Molecular weight	Qualitation ion (*m/z*)
99	Hydroxyvardenafil	$C_{23}H_{32}N_6O_5S$	504	—
100	Ibuprofen	$C_{13}H_{18}O_2$	206	206, 161, 117, 91, 65
101	Imidazosagatriazinone	$C_{17}H_{20}N_4O_2$	312	312, 284, 136,240
102	Indomethacin	$C_{19}H_{16}ClNO_4$	357	139, 313, 111, 75
103	Ketoconazole	$C_{26}H_{28}Cl_2N_4O_4$	530	—
104	Ketoprofen	$C_{16}H_{14}O_3$	254	105, 177, 209, 77, 254, 45, 194, 131, 165
105	Lidocaine	$C_{14}H_{22}N_2O$	234	234, 120, 86, 58
106	Liothyronine	$C_{15}H_{12}I_3NO_4$	651	—
107	Lorazepam	$C_{15}H_{10}Cl_2N_2O_2$	320	239, 274, 302, 75, 138, 177, 111, 203, 163, 100
108	Mazindol	$C_{16}H_{13}ClN_2O$	284	266, 231, 204, 176, 128, 102, 75
109	Mefenamic acid	$C_{15}H_{15}NO_2$	241	241, 223, 180, 152, 102
110	Melatonin	$C_{13}H_{16}N_2O_2$	232	232, 172, 160, 145, 130, 117, 102, 89
111	Mephenesin	$C_{10}H_{14}O_3$	182	182, 108, 91
112	Mephentermine	$C_{11}H_{17}N$	163	72, 91, 148, 56, 42, 115
113	Meprobamate	$C_9H_{18}N_2O_4$	218	83, 55, 43, 71, 62, 96, 114, 144, 101
114	Metformin	$C_4H_{11}N_5$	129	—
115	Methamphetamine	$C_{10}H_{15}N$	149	58, 91, 65, 134, 42, 115, 119
116	Methandriol	$C_{20}H_{32}O_2$	304	253, 213, 271, 304, 105, 145, 286, 228, 119, 159
117	Methandrostenolone	$C_{20}H_{28}O_2$	300	122, 91, 161, 147, 105, 134, 77
118	Methaqualone	$C_{16}H_{14}N_2O$	250	250, 91, 132, 65, 77, 217, 117, 50, 104
119	Metharbital	$C_9H_{14}N_2O_3$	198	155, 112, 83, 55
120	Methimazole	$C_4H_6N_2S$	114	114, 72, 81, 42, 54, 86, 59
121	Methylprednisolone	$C_{22}H_{30}O_5$	374	136, 91, 55
122	Methyltestosterone	$C_{20}H_{30}O_2$	302	302, 229, 202, 161, 124, 91
123	Metoclopramide	$C_{14}H_{22}ClN_3O_2$	299	184, 86, 58
124	Metronidazole	$C_6H_9N_3O_3$	171	171, 124, 81, 53
125	Minoxidil	$C_9H_{15}N_5O$	209	193, 164, 138, 110, 84, 67
126	Morphine	$C_{17}H_{19}NO_3$	285	285, 162, 42, 215, 115, 55, 65, 92, 81
127	Nalidixic acid	$C_{12}H_{12}N_2O_3$	232	188, 160, 132, 173, 145, 104, 232, 77
128	Nandrolone	$C_{18}H_{26}O_2$	274	274, 215, 173, 147, 119, 91, 67
129	Naproxen	$C_{14}H_{14}O_3$	230	230, 185, 170, 141, 115
130	Nicametate	$C_{12}H_{18}N_2O_2$	222	—

Published, Nov 23, 2012
Revised, Feb 17, 2014
Revised, March 5, 2020
TFDAO0015.02

NO.	Compound	Molecular formula	Molecular weight	Qualitation ion (*m/z*)
131	Nifedipine	$C_{17}H_{18}N_2O_6$	346	329, 284, 224, 268, 254, 195, 180
132	Nitrofurantoin	$C_8H_6N_4O_5$	238	—
133	Noracetildenafil	$C_{24}H_{32}N_6O_3$	452	113, 70, 42, 56, 98, 207, 311, 452, 136, 354
134	Norethisterone	$C_{20}H_{26}O_2$	298	298, 283, 265
135	Norfloxacin	$C_{16}H_{18}FN_3O_3$	319	—
136	Norneosildenafil	$C_{22}H_{29}N_5O_4S$	459	—
137	Nortadalafil	$C_{21}H_{17}N_3O_4$	375	—
138	Nylidrin	$C_{19}H_{25}NO_2$	299	—
139	Orlistat	$C_{29}H_{53}NO_5$	495	292, 114, 69, 96, 55, 82
140	Orphenadrine	$C_{18}H_{23}NO$	269	58, 73, 165, 178, 45
141	Oxethazaine	$C_{28}H_{41}N_3O_3$	467	114, 86, 213, 56, 133, 72, 304
142	Oxymetholone	$C_{21}H_{32}O_3$	332	174, 275, 332, 43, 161, 91, 81, 71, 216, 107
143	Oxyphenbutazone	$C_{19}H_{20}N_2O_3$	324	93, 45, 55, 69, 161, 193, 77, 249
144	Oxyphencyclimine	$C_{20}H_{28}N_2O_3$	344	—
145	Pentazocine	$C_{19}H_{27}NO$	285	217, 202, 285, 110, 270, 70, 45, 159, 173
146	Phenacetin	$C_{10}H_{13}NO_2$	179	179, 137, 108, 80, 65, 53
147	Phenazopyridine	$C_{11}H_{11}N_5$	213	213, 108, 81, 54, 136, 97, 184, 66, 155
148	Phenformin	$C_{10}H_{15}N_5$	205	146, 104.91, 77, 65
149	Phenobarbital	$C_{12}H_{12}N_2O_3$	232	204, 117, 232, 161, 146, 103, 77, 91, 174
150	Phenolphthalein	$C_{20}H_{14}O_4$	318	318, 274, 225, 181, 152, 152, 104, 65
151	Phentermine	$C_{10}H_{15}N$	149	70, 91, 105, 58, 65, 115, 41, 115
152	Phentolamine	$C_{17}H_{19}N_3O$	281	199, 183, 91, 154, 77, 128, 170
153	Phenylbutazone	$C_{19}H_{20}N_2O_2$	308	308, 252, 183, 152, 105, 77
154	Phenylephrine	$C_9H_{13}NO_2$	167	135, 44, 107, 179, 160, 77, 51, 91
155	Phenylpropanolamine	$C_9H_{13}NO$	151	44, 77, 105, 51, 117, 91
156	Pioglitazone	$C_{19}H_{20}N_2O_3S$	356	—
157	Piperiacetildenafil	$C_{24}H_{31}N_5O_3$	437	—
158	Piperidenafil	$C_{22}H_{29}N_5O_4S$	459	431, 459, 283, 67, 42, 84, 121, 135, 149, 215
159	Pirenzepine	$C_{19}H_{21}N_5O_2$	351	351, 281, 211, 113, 70
160	Piroxicam	$C_{15}H_{13}N_3O_4S$	331	104, 76, 43, 152, 169, 118, 386, 211, 91

Published, Nov 23, 2012
Revised, Feb 17, 2014
Revised, March 5, 2020
TFDAO0015.02

NO.	Compound	Molecular formula	Molecular weight	Qualitation ion (*m/z*)
161	Prednisolone	$C_{21}H_{28}O_5$	360	122, 91, 55
162	Prednisone	$C_{21}H_{26}O_5$	358	298, 245, 226, 186, 160, 131, 115, 91
163	Primidone	$C_{12}H_{14}N_2O_2$	218	146, 190, 117, 161, 103, 91, 77, 174
164	Probenecid	$C_{13}H_{19}NO_4S$	285	270, 135, 199, 104, 76, 43
165	Procaine	$C_{13}H_{20}N_2O_2$	236	86, 99, 120, 65, 56, 164
166	Progesterone	$C_{21}H_{30}O_2$	314	314, 272, 229, 147, 124, 91, 67
167	Propantheline	$C_{23}H_{30}NO_3^+$	368	86, 181, 310, 99, 152, 44, 58, 325, 127, 71
168	Propranolol	$C_{16}H_{21}NO_2$	259	259, 215, 144, 115, 72
169	Quinine	$C_{20}H_{24}N_2O_2$	324	189, 160, 136
170	Ranitidine	$C_{13}H_{22}N_4O_3$	314	235, 137, 94, 67
171	Reserpine	$C_{33}H_{40}N_2O_9$	608	—
172	Rimonabant	$C_{22}H_{21}Cl_3N_4O$	462	84, 363, 55, 99, 282, 335, 299, 41, 380, 145,462
173	Rosiglitazone	$C_{18}H_{19}N_3O_3S$	357	—
174	Salicylamide	$C_7H_7NO_2$	137	120, 137, 92, 65, 53, 44, 80
175	Salicylic acid	$C_7H_6O_3$	138	120, 92, 138, 64, 46
176	Scopolamine	$C_{17}H_{21}NO_4$	303	94, 138, 108, 154, 303
177	Secobarbital	$C_{12}H_{18}N_2O_3$	238	195, 168, 124, 97, 53
178	Sibutramine	$C_{17}H_{26}ClN$	279	114, 72, 58, 101, 128, 137
179	Sildenafil	$C_{22}H_{30}N_6O_4S$	474	404, 281, 207, 99, 56
180	Stanozolol	$C_{21}H_{32}N_2O$	328	96, 328, 257, 270, 133, 119, 175
181	Strychnine	$C_{21}H_{22}N_2O_2$	334	334, 167, 130, 107, 77, 55
182	Sulfadiazine	$C_{10}H_{10}N_4O_2S$	250	185, 92, 65, 108
183	Sulfadimethoxine	$C_{12}H_{14}N_4O_4S$	310	259, 140, 92, 65, 168, 108, 121, 82, 187
184	Sulfamerazine	$C_{11}H_{12}N_4O_2S$	264	199, 92, 65
185	Sulfamethazine	$C_{12}H_{14}N_4O_2S$	278	213, 92, 65
186	Sulfamethizole	$C_9H_{10}N_4O_2S_2$	270	—
187	Sulfamethoxazole	$C_{10}H_{11}N_3O_3S$	253	238, 224, 42, 206, 165, 266, 72, 91, 56
188	Sulfamethoxypyridazine	$C_{11}H_{12}N_4O_3S$	280	215, 92, 108, 65, 53, 80, 280
189	Sulfanilamide	$C_6H_8N_2O_2S$	172	172, 92, 65
190	Sulfathiazole	$C_9H_9N_3O_2S_2$	255	—
191	Sulfinpyrazone	$C_{23}H_{20}N_2O_3S$	404	278, 249, 209, 183, 152, 130, 105, 77, 51
192	Sulfisoxazole	$C_{11}H_{13}N_3O_3S$	267	—
193	Sulindac	$C_{20}H_{17}FO_3S$	356	233, 297, 312, 248, 67, 123, 47, 133, 220

NO.	Compound	Molecular formula	Molecular weight	Qualitation ion (*m/z*)
194	Synephrine	$C_9H_{13}NO_2$	167	135, 44, 107, 179, 160, 77, 51, 91
195	Tadalafil	$C_{22}H_{19}N_3O_4$	389	389, 262, 204, 169
196	Terbinafine	$C_{21}H_{25}N$	291	141, 276, 234, 115, 291, 196
197	Terfenadine	$C_{32}H_{41}NO_2$	471	—
198	Testosterone	$C_{19}H_{28}O_2$	288	288, 246, 203, 147, 124, 91, 55
199	Tetracaine	$C_{15}H_{24}N_2O_2$	264	58, 71, 176, 150, 105, 193, 92
200	Theobromine	$C_7H_8N_4O_2$	180	180, 67, 109, 55, 82, 137, 42, 94
201	Theophylline	$C_7H_8N_4O_2$	180	180, 95, 68, 53
202	Thiodimethylsildenafil	$C_{23}H_{32}N_6O_3S_2$	504	113, 70, 42, 84, 328, 343, 56
203	Thiohomosildenafil	$C_{23}H_{32}N_6O_3S_2$	504	113, 70, 56, 475, 98, 42, 327, 341, 269, 84
204	Thioridazine	$C_{21}H_{26}N_2S_2$	370	370, 244, 185, 126, 98, 70
205	Thiosildenafil	$C_{22}H_{30}N_6O_3S_2$	490	99, 448, 56, 489, 425, 70, 207
206	Tinidazole	$C_8H_{13}N_3O_4S$	247	201, 123, 80, 68, 93, 107, 53, 154, 247
207	Tolbutamide	$C_{12}H_{18}N_2O_3S$	270	91, 171, 155, 65, 107, 77, 197
208	Triamcinolone	$C_{21}H_{27}FO_6$	394	—
209	Vardenafil	$C_{23}H_{32}N_6O_4S$	488	—
210	Desulfovardenafil (Vardenafil analogue 【2-(2-ethoxy-phenyl)-5-methyl-7-propyl-3H-imidazo(51-f)-(1,2,4)triazin-4-one】)	$C_{17}H_{20}N_4O_2$	312	284, 312, 256, 67, 297, 120, 269, 93, 135
211	Xanthinol Niacinate	$C_{13}H_{21}N_5O_4$	311	—
212	Yohimbine	$C_{21}H_{26}N_2O_3$	354	353, 169
213	Zolpidem	$C_{19}H_{21}N_3O$	307	235, 207, 219, 281, 307, 65, 92, 191
214	Cetilistat	$C_{25}H_{39}NO_3$	401	177, 160, 133, 55, 104, 77, 401
215	Avanafil	$C_{23}H_{26}ClN_7O_3$	483	—
216	Benproperine	$C_{21}H_{27}NO$	309	112, 165, 91
217	Celecoxib	$C_{17}H_{14}F_3N_3O_2S$	381	381, 300, 281
218	Clozapine	$C_{18}H_{19}ClN_4$	326	243, 256, 192, 326
219	Cyproheptadine	$C_{21}H_{21}N$	287	215, 287, 96, 189
220	Desacetyl bisacodyl	$C_{18}H_{15}NO_2$	277	277, 276, 199

NO.	Compound	Molecular formula	Molecular weight	Qualitation ion (*m/z*)
221	2-Diphenylmethylpyrrolidine (Desoxy-D2PM)	$C_{17}H_{19}N$	237	70, 165
222	Famotidine	$C_8H_{15}N_7O_2S_3$	337	—
223	Hydroxyzine	$C_{21}H_{27}ClN_2O_2$	374	201, 165, 299
224	Lorcaserin	$C_{11}H_{14}ClN$	195	153, 115, 195, 166
225	Nefopam	$C_{17}H_{19}NO$	253	179, 58, 165, 225
226	Norgestrel	$C_{21}H_{28}O_2$	312	91, 245, 79, 312
227	Omeprazole	$C_{17}H_{19}N_3O_3S$	345	296, 329, 281
228	Prilocaine	$C_{13}H_{20}N_2O$	220	86, 106, 107
229	Promethazine	$C_{17}H_{20}N_2S$	284	72, 180, 284
230	Spironolactone	$C_{24}H_{32}O_4S$	416	267, 340
231	Topiramate	$C_{12}H_{21}NO_8S$	339	245, 69, 127, 171
232	Trimethoprim	$C_{14}H_{18}N_4O_3$	290	290, 259, 275, 123

Note: 1. Ionization: Electron ionization (EI).

2. Collision energy: 70 eV.

3. " — " represents that compound cannot be detected by GC-MS.

4. All the parameters can be adjusted depending on the instruments used if the above conditions are not applicable.

Published, Nov 23, 2012
Revised, Feb 17, 2014
Revised, March 5, 2020
TFDAO0015.02

Table 4. The parameters of 232 medicines analyzed by LC-MS/MS

NO.	Compound	Molecular formula	Molecular weight	Ionization mode	Cone voltage (V)	Collision energy (eV)	Precursor ion (*m/z*)	Product ion (*m/z*)
1	Acetaminophen	$C_8H_9NO_2$	151	ESI^+	40	26	152	110, 94
2	Acetil acid	$C_{18}H_{20}N_4O_4$	356	ESI^+	40	25	357	329, 285, 300
3	Acetildenafil	$C_{25}H_{34}N_6O_3$	466	ESI^+	50	40	467	127, 111, 84, 72
4	Acetohexamide	$C_{15}H_{20}N_2O_4S$	324	ESI^+	40	25	347	222, 302, 248, 122
5	Acetylvardenafil	$C_{25}H_{34}N_6O_3$	466	ESI^+	30	35	467	341, 151, 107, 166, 317
6	Allopurinol	$C_5H_4N_4O$	136	ESI^+	40	21	137	110, 94, 54, 120, 81
7	Aminopyrine	$C_{13}H_{17}N_3O$	231	ESI^+	30	20	232	113, 98, 72
8	Aminotadalafil	$C_{21}H_{18}N_4O_4$	390	ESI^+	60	25	391	135, 286, 150
9	Amitriptyline	$C_{20}H_{23}N$	277	ESI^+	30	20	278	91, 233, 105, 117, 155, 191, 218, 84
10	Amphetamine	$C_9H_{13}N$	135	ESI^+	15	8	136	119, 91
11	Aspirin	$C_9H_8O_4$	180	ESI^-	8	2	179	137
12	Atenolol	$C_{14}H_{22}N_2O_3$	266	ESI^+	30	21	267	145, 190, 74, 72, 225, 208, 178, 116
13	Atropine	$C_{17}H_{23}NO_3$	289	ESI^+	35	21	290	124, 93
14	Barbital	$C_8H_{12}N_2O_3$	184	ESI^-	25	15	183	42, 140, 96, 85
15	Benzbromarone	$C_{17}H_{12}Br_2O_3$	424	ESI^-	45	29	423	251, 407, 81, 278
16	Benzhexol	$C_{20}H_{31}NO$	301	ESI^+	30	10	302	98
17	Benzocaine	$C_9H_{11}NO_2$	165	ESI^+	20	17	166	138, 120, 94
18	Betamethasone	$C_{22}H_{29}FO_5$	392	ESI^+	20	10	393	393, 355, 309, 337, 279
19	Bezafibrate	$C_{19}H_{20}ClNO_4$	361	ESI^+	15	15	362	276, 362
20	Bisacodyl	$C_{22}H_{19}NO_4$	361	ESI^+	30	20	362	184, 226
21	Bromhexine	$C_{14}H_{20}Br_2N_2$	376	ESI^+	30	18	377	264, 114
22	Brompheniramine	$C_{16}H_{19}BrN_2$	318	ESI^+	30	8	319	274
23	Bromvalerylurea	$C_6H_{11}BrN_2O_2$	222	ESI^+	30	15	223	223, 163

Published, Nov 23, 2012
Revised, Feb 17, 2014
Revised, March 5, 2020
TFDAO0015.02

NO.	Compound	Molecular formula	Molecular weight	Ionization mode	Cone voltage (V)	Collision energy (eV)	Precursor ion (*m/z*)	Product ion (*m/z*)
24	Bucetin	$C_{12}H_{17}NO_3$	223	ESI^+	20	15	224	138, 164, 206
25	Butropium	$C_{28}H_{38}NO_4^+$	452	ESI^+	45	35	453	163, 288, 349
26	Caffeine	$C_8H_{10}N_4O_2$	194	ESI^+	40	32	195	138
27	Camylofine	$C_{19}H_{32}N_2O_2$	320	ESI^+	40	20	321	100, 72, 135, 178, 248
28	Carbetapentane	$C_{20}H_{31}NO_3$	333	ESI^+	40	18	334	100, 145, 217
29	Carbimazole	$C_7H_{10}O_2N_2S$	186	ESI^+	20	15	187	115, 143, 159
30	Carbinoxamine	$C_{16}H_{19}ClN_2O$	290	ESI^+	25	15	291	202, 167, 72
31	Carbodenafil	$C_{24}H_{32}N_6O_3$	452	ESI^+	50	23	453	339, 311
32	Carisoprodol	$C_{12}H_{24}N_2O_4$	260	ESI^+	30	20	261	97, 62, 176, 158
33	Chloramphenicol	$C_{11}H_{12}Cl_2N_2O_5$	322	ESI^+	20	10	323	305, 275, 241
34	Chlordiazepoxide	$C_{16}H_{14}ClN_3O$	299	ESI^+	30	20	300	227, 283, 241, 255
35	Chlormezanone	$C_{11}H_{12}ClNO_3S$	273	ESI^-	25	20	272	208, 180, 152, 71
36	Chloropretadalafil	$C_{22}H_{19}ClN_2O_5$	426	ESI^+	30	14	427	135, 334, 395, 262
37	Chlorothiazide	$C_7H_6ClN_3O_4S_2$	295	ESI^+	15	15	296	278, 221, 205
38	Chlorpheniramine	$C_{16}H_{19}ClN_2$	274	ESI^+	20	15	275	230
39	Chlorpromazine	$C_{17}H_{19}ClN_2S$	318	ESI^+	40	20	319	86, 58, 239, 246, 274
40	Chlorpropamide	$C_{10}H_{13}ClN_2O_3S$	276	ESI^-	30	17	275	190
41	Chlorzoxazone	$C_7H_4ClNO_2$	169	ESI^+	50	3	170	114, 142
42	Cimetidine	$C_{10}H_{16}N_6S$	252	ESI^+	30	15	253	159, 117, 95, 172, 211
43	Cinnarizine	$C_{26}H_{28}N_2$	368	ESI^+	30	15	369	167, 201
44	Clobenzorex	$C_{16}H_{18}ClN$	259	ESI^+	30	20	260	91, 119, 125, 142
45	Clofibrate	$C_{12}H_{15}ClO_3$	242	ESI^+	25	10	243	87, 169, 197, 115
46	Cocaine	$C_{17}H_{21}NO_4$	303	ESI^+	35	25	304	182
47	Colchicine	$C_{22}H_{25}O_6N$	399	ESI^+	50	40	400	310, 358, 282, 298
48	Cortisone	$C_{21}H_{28}O_5$	360	ESI^-	30	3	359	137, 311, 329

Published, Nov 23, 2012
Revised, Feb 17, 2014
Revised, March 5, 2020
TFDAO0015.02

NO.	Compound	Molecular formula	Molecular weight	Ionization mode	Cone voltage (V)	Collision energy (eV)	Precursor ion (*m/z*)	Product ion (*m/z*)
49	7-Ketodehydroepiandrosterone (7-keto-DHEA)	$C_{19}H_{26}O_3$	302	ESI^-	20	12	301	283, 245
50	*N*-Desethylvardenafil	$C_{21}H_{28}N_6O_4S$	460	ESI^+	45	30	461	151, 312, 284, 85, 376
51	*N*-Desethylacetildenafil	$C_{23}H_{30}N_6O_3$	438	ESI^+	50	27	439	99, 339, 353
52	*N*-Desmethylsibutramine	$C_{16}H_{24}ClN$	265	ESI^+	25	20	266	139, 125, 153
53	*N*-Desmethylsildenafil	$C_{21}H_{28}N_6O_4S$	460	ESI^+	45	29	461	85, 311, 283, 377
54	*N*-Didesmethylsibutramine	$C_{15}H_{22}ClN$	251	ESI^+	20	13	252	139, 125, 153, 179, 97
55	Dexamethasone	$C_{22}H_{29}FO_5$	392	ESI^-	30	20	391	361
56	Dextromethorphan	$C_{18}H_{25}NO$	271	ESI^+	35	35	272	147, 213, 215, 121
57	Diazepam	$C_{16}H_{13}ClN_2O$	284	ESI^+	50	35	285	222, 193, 154
58	Dibucaine	$C_{20}H_{29}N_3O_2$	343	ESI^+	40	25	344	271, 215
59	Diclofenac	$C_{14}H_{11}Cl_2NO_2$	295	ESI^-	10	12	294	250
60	Dicyclomine	$C_{19}H_{35}NO_2$	309	ESI^+	30	25	310	165, 237, 155, 109, 100
61	Diethylpropion	$C_{13}H_{19}NO$	205	ESI^+	30	20	206	105, 100, 133, 72
62	Diethylstilbestrol	$C_{18}H_{20}O_2$	268	ESI^-	50	27	267	251, 237, 222, 223, 209, 93
63	Digitoxin	$C_{41}H_{64}O_{13}$	764	ESI^-	60	10	763	133, 85
64	Dimethylsildenafil	$C_{23}H_{32}N_6O_4S$	488	ESI^+	50	29	489	113, 99, 71, 311, 283, 377
65	Diphenhydramine	$C_{17}H_{21}NO$	255	ESI^+	20	8	256	167
66	Diphenylhydantoin	$C_{15}H_{12}N_2O_2$	252	ESI^+	30	10	253	182, 104
67	Diprophylline	$C_{10}H_{14}N_4O_4$	254	ESI^+	30	19	255	181, 124
68	Dipyridamole	$C_{24}H_{40}N_8O_4$	504	ESI^+	50	42	505	429, 385
69	Econazole	$C_{18}H_{15}Cl_3N_2O$	380	ESI^+	40	20	381	125, 193, 69
70	Estradiol	$C_{18}H_{24}O_2$	272	ESI^-	30	40	271	145, 183, 239
71	Estriol	$C_{18}H_{24}O_3$	288	ESI^-	40	50	287	145, 171
72	Estrone	$C_{18}H_{22}O_2$	270	ESI^-	50	45	269	145, 159
73	Ethinylestradiol	$C_{20}H_{24}O_2$	296	ESI^-	60	40	295	145, 159, 183

Published, Nov 23, 2012
Revised, Feb 17, 2014
Revised, March 5, 2020
TFDAO0015.02

NO.	Compound	Molecular formula	Molecular weight	Ionization mode	Cone voltage (V)	Collision energy (eV)	Precursor ion (*m/z*)	Product ion (*m/z*)
74	Ethisterone	$C_{21}H_{28}O_2$	312	ESI^+	35	20	313	97, 109
75	Ethoxybenzamide	$C_9H_{11}NO_2$	165	ESI^+	25	16	166	149, 121
76	Ethylestrenol	$C_{20}H_{32}O$	288	ESI^+	25	3	289	270
77	Etofibrate	$C_{18}H_{18}ClNO_5$	363	ESI^+	30	15	364	150, 169, 113, 236
78	Fenfluramine	$C_{12}H_{16}F_3N$	231	ESI^+	20	13	232	159, 187
79	Fenofibrate	$C_{20}H_{21}ClO_4$	360	ESI^+	40	15	361	233, 139
80	Finasteride	$C_{23}H_{36}N_2O_2$	372	ESI^+	50	32	373	305, 317, 95, 69, 57
81	Flavoxate	$C_{24}H_{25}NO_4$	391	ESI^+	30	17	392	112, 307, 263
82	Fluoxetine	$C_{17}H_{18}F_3NO$	309	ESI^+	30	20	310	259, 148, 70, 105, 117, 231
83	Fluoxymesterone	$C_{20}H_{29}FO_3$	336	ESI^+	50	40	337	131
84	Furosemide	$C_{12}H_{11}ClN_2O_5S$	330	ESI^-	10	20	329	285, 205
85	Gemfibrozil	$C_{15}H_{22}O_3$	250	ESI^-	25	8	249	121, 127
86	Gendenafil	$C_{19}H_{22}N_4O_3$	354	ESI^+	45	25	355	327, 285, 297
87	Glibenclamide	$C_{23}H_{28}ClN_3O_5S$	493	ESI^-	50	26	492	170, 367, 378, 460
88	Glycopyrronium	$C_{19}H_{28}NO_3^+$	317	ESI^+	35	3	318	116, 58, 88
89	Griseofulvin	$C_{17}H_{17}ClO_6$	352	ESI^+	35	18	353	165, 285, 215, 69
90	Guaifenesin	$C_{10}H_{14}O_4$	198	ESI^+	20	7	199	163, 125, 181, 151
91	Homatropine	$C_{16}H_{21}NO_3$	275	ESI^+	40	23	276	124, 142, 93
92	Homosildenafil	$C_{23}H_{32}N_6O_4S$	488	ESI^+	60	37	489	283, 113, 72
93	Hydralazine	$C_8H_8N_4$	160	ESI^+	35	16	161	89, 116, 132, 145
94	Hydrochlorothiazide	$C_7H_8ClN_3O_4S_2$	297	ESI^-	40	27	296	269, 205
95	Hydrocortisone	$C_{21}H_{30}O_5$	362	ESI^+	35	20	363	121, 309, 267, 241, 187, 147
96	Hydroxyacetildenafil	$C_{25}H_{34}N_6O_4$	482	ESI^+	50	40	483	143, 127, 112, 97
97	Hydroxyhomosildenafil	$C_{23}H_{32}N_6O_5S$	504	ESI^+	60	35	505	487, 112, 99
98	Hydroxythiohomosildenafil	$C_{23}H_{32}N_6O_4S_2$	520	ESI^+	50	30	521	99, 503, 327, 299, 129, 112
99	Hydroxyvardenafil	$C_{23}H_{32}N_6O_5S$	504	ESI^+	50	35	505	151, 99, 312, 299, 376

Published, Nov 23, 2012
Revised, Feb 17, 2014
Revised, March 5, 2020
TFDAO0015.02

NO.	Compound	Molecular formula	Molecular weight	Ionization mode	Cone voltage (V)	Collision energy (eV)	Precursor ion (*m/z*)	Product ion (*m/z*)
100	Ibuprofen	$C_{13}H_{18}O_2$	206	ESI^-	20	6	205	161, 159
101	Imidazosagatriazinone	$C_{17}H_{20}N_4O_2$	312	ESI^+	40	24	313	285, 256, 166
102	Indomethacin	$C_{19}H_{16}ClNO_4$	357	ESI^+	30	15	358	139, 174
103	Ketoconazole	$C_{26}H_{28}Cl_2N_4O_4$	530	ESI^+	50	40	531	82, 489, 255, 244, 177, 112
104	Ketoprofen	$C_{16}H_{14}O_3$	254	ESI^+	30	15	255	209, 105, 177
105	Lidocaine	$C_{14}H_{22}N_2O$	234	ESI^-	40	25	233	215, 143, 120
106	Liothyronine	$C_{15}H_{12}I_3NO_4$	651	ESI^+	40	20	652	606, 508, 635
107	Lorazepam	$C_{15}H_{10}Cl_2N_2O_2$	320	ESI^+	30	15	321	275, 320
108	Mazindol	$C_{16}H_{13}ClN_2O$	284	ESI^+	35	19	285	44
109	Mefenamic acid	$C_{15}H_{15}NO_2$	241	ESI^+	20	15	242	224
110	Melatonin	$C_{13}H_{16}N_2O_2$	232	ESI^+	30	11	233	174, 216
111	Mephenesin	$C_{10}H_{14}O_3$	182	ESI^+	20	10	183	147, 135, 109, 121, 165
112	Mephentermine	$C_{11}H_{17}N$	163	ESI^+	20	15	164	133, 91
113	Meprobamate	$C_9H_{18}N_2O_4$	218	ESI^+	15	5	219	158, 97
114	Metformin	$C_4H_{11}N_5$	129	ESI^+	25	20	130	60, 71, 85, 88, 113
115	Methamphetamine	$C_{10}H_{15}N$	149	ESI^+	20	11	150	91, 119
116	Methandriol	$C_{20}H_{32}O_2$	304	ESI^+	30	20	305	270, 214
117	Methandrostenolone	$C_{20}H_{28}O_2$	300	ESI^+	30	13	301	149, 283, 121
118	Methaqualone	$C_{16}H_{14}N_2O$	250	ESI^+	40	26	251	132, 91, 161
119	Metharbital	$C_9H_{14}N_2O_3$	198	ESI^-	25	20	197	42
120	Methimazole	$C_4H_6N_2S$	114	ESI^+	30	26	115	57, 81, 88, 100, 82, 83, 56
121	Methylprednisolone	$C_{22}H_{30}O_5$	374	ESI^+	50	35	375	135, 357, 161
122	Methyltestosterone	$C_{20}H_{30}O_2$	302	ESI^+	40	25	303	109, 97
123	Metoclopramide	$C_{14}H_{22}ClN_3O_2$	299	ESI^+	30	15	300	227, 184
124	Metronidazole	$C_6H_9N_3O_3$	171	ESI^+	25	17	172	128, 82, 111, 56
125	Minoxidil	$C_9H_{15}N_5O$	209	ESI^+	30	16	210	193, 164, 137, 110, 84

Published, Nov 23, 2012
Revised, Feb 17, 2014
Revised, March 5, 2020
TFDAO0015.02

NO.	Compound	Molecular formula	Molecular weight	Ionization mode	Cone voltage (V)	Collision energy (eV)	Precursor ion (*m/z*)	Product ion (*m/z*)
126	Morphine	$C_{17}H_{19}NO_3$	285	ESI^+	30	20	286	165, 153, 181, 209
127	Nalidixic acid	$C_{12}H_{12}N_2O_3$	232	ESI^+	25	10	233	215
128	Nandrolone	$C_{18}H_{26}O_2$	274	ESI^+	35	22	275	109, 257, 239, 83
129	Naproxen	$C_{14}H_{14}O_3$	230	ESI^+	15	15	231	185, 170
130	Nicametate	$C_{12}H_{18}N_2O_2$	222	ESI^+	20	12	223	150, 106, 78, 100
131	Nifedipine	$C_{17}H_{18}N_2O_6$	346	ESI^+	35	25	347	195, 223, 167, 253, 270
132	Nitrofurantoin	$C_8H_6N_4O_5$	238	ESI^+	30	15	239	222, 95, 122, 168, 67
133	Noracetildenafil	$C_{24}H_{32}N_6O_3$	452	ESI^+	50	30	453	97, 113, 453, 70, 325, 353, 297, 396
134	Norethisterone	$C_{20}H_{26}O_2$	298	ESI^+	30	15	299	109, 299, 231, 135
135	Norfloxacin	$C_{16}H_{18}FN_3O_3$	319	ESI^+	30	15	320	302, 233, 276, 205
136	Norneosildenafil	$C_{22}H_{29}N_5O_4S$	459	ESI^+	50	35	460	283, 299, 311, 256, 84
137	Nortadalafil	$C_{21}H_{17}N_3O_4$	375	ESI^+	30	20	376	276, 254, 135, 262, 302
138	Nylidrin	$C_{19}H_{25}NO_2$	299	ESI^+	40	25	300	150, 91, 133, 105, 282
139	Orlistat	$C_{29}H_{53}NO_5$	495	ESI^-	40	14	494	158, 140, 266, 451
140	Orphenadrine	$C_{18}H_{23}NO$	269	ESI^+	20	6	270	181
141	Oxethazaine	$C_{28}H_{41}N_3O_3$	467	ESI^+	40	18	468	145, 204, 277, 336
142	Oxymetholone	$C_{21}H_{32}O_3$	332	ESI^+	30	10	333	187, 223, 239
143	Oxyphenbutazone	$C_{19}H_{20}N_2O_3$	324	ESI^+	35	17	325	160, 162, 176, 227, 297
144	Oxyphencyclimine	$C_{20}H_{28}N_2O_3$	344	ESI^+	40	18	345	129
145	Pentazocine	$C_{19}H_{27}NO$	285	ESI^+	30	20	286	218, 69, 159, 175
146	Phenacetin	$C_{10}H_{13}NO_2$	179	ESI^+	40	25	180	110, 138
147	Phenazopyridine	$C_{11}H_{11}N_5$	213	ESI^+	40	18	214	122, 77, 93
148	Phenformin	$C_{10}H_{15}N_5$	205	ESI^+	30	23	206	60, 105, 164
149	Phenobarbital	$C_{12}H_{12}N_2O_3$	232	ESI^-	20	14	231	42, 188, 85
150	Phenolphthalein	$C_{20}H_{14}O_4$	318	ESI^-	43	3	317	93, 265, 169

Published, Nov 23, 2012
Revised, Feb 17, 2014
Revised, March 5, 2020
TFDAO0015.02

NO.	Compound	Molecular formula	Molecular weight	Ionization mode	Cone voltage (V)	Collision energy (eV)	Precursor ion (*m/z*)	Product ion (*m/z*)
151	Phentermine	$C_{10}H_{15}N$	149	ESI^+	15	9	150	133, 91
152	Phentolamine	$C_{17}H_{19}N_3O$	281	ESI^-	40	21	280	133, 120, 161, 197, 210
153	Phenylbutazone	$C_{19}H_{20}N_2O_2$	308	ESI^-	30	26	307	279, 131, 160
154	Phenylephrine	$C_9H_{13}NO_2$	167	ESI^+	20	11	168	150
155	Phenylpropanolamine	$C_9H_{13}NO$	151	ESI^+	19	11	152	134
156	Pioglitazone	$C_{19}H_{20}N_2O_3S$	356	ESI^-	30	30	355	312, 150, 178, 115, 284
157	Piperiacetildenafil	$C_{24}H_{31}N_5O_3$	437	ESI^+	50	26	438	98
158	Piperidenafil	$C_{22}H_{29}N_5O_4S$	459	ESI^+	50	30	460	151, 284, 312
159	Pirenzepine	$C_{19}H_{21}N_5O_2$	351	ESI^+	40	16	352	113, 252, 141, 70
160	Piroxicam	$C_{15}H_{13}N_3O_4S$	331	ESI^+	34	26	332	95
161	Prednisolone	$C_{21}H_{28}O_5$	360	ESI^+	20	12	361	147, 325, 307, 265, 361, 343
162	Prednisone	$C_{21}H_{26}O_5$	358	ESI^+	25	14	359	341, 313, 267, 147, 93, 213, 171
163	Primidone	$C_{12}H_{14}N_2O_2$	218	ESI^+	20	12	219	162, 119, 174
164	Probenecid	$C_{13}H_{19}NO_4S$	285	ESI^-	30	13	284	240, 141, 198, 164
165	Procaine	$C_{13}H_{20}N_2O_2$	236	ESI^+	25	15	237	164, 120, 100
166	Progesterone	$C_{21}H_{30}O_2$	314	ESI^+	40	16	315	97, 109, 297, 85
167	Propantheline	$C_{23}H_{30}NO_3^+$	368	ESI^+	40	19	369	100, 181, 326, 253
168	Propranolol	$C_{16}H_{21}NO_2$	259	ESI^+	35	25	260	116, 183, 157, 98, 74, 72
169	Quinine	$C_{20}H_{24}N_2O_2$	324	ESI^+	50	27	325	81, 307, 184, 160, 253, 110, 264
170	Ranitidine	$C_{13}H_{22}N_4O_3$	314	ESI^+	30	14	315	176, 270, 124, 144, 224
171	Reserpine	$C_{33}H_{40}N_2O_9$	608	ESI^+	65	28	609	195, 397, 174, 448
172	Rimonabant	$C_{22}H_{21}Cl_3N_4O$	462	ESI^+	50	25	463	363, 84
173	Rosiglitazone	$C_{18}H_{19}N_3O_3S$	357	ESI^+	50	33	358	135
174	Salicylamide	$C_7H_7NO_2$	137	ESI^-	25	15	136	118, 93, 91
175	Salicylic acid	$C_7H_6O_3$	138	ESI^-	25	11	137	93
176	Scopolamine	$C_{17}H_{21}NO_4$	303	ESI^+	30	25	304	138, 121, 186, 110, 98

Published, Nov 23, 2012
Revised, Feb 17, 2014
Revised, March 5, 2020
TFDAO0015.02

NO.	Compound	Molecular formula	Molecular weight	Ionization mode	Cone voltage (V)	Collision energy (eV)	Precursor ion (*m/z*)	Product ion (*m/z*)
177	Secobarbital	$C_{12}H_{18}N_2O_3$	238	ESI^-	25	16	237	42, 194, 85, 150
178	Sibutramine	$C_{17}H_{26}ClN$	279	ESI^+	40	18	280	179, 153, 139, 125, 97
179	Sildenafil	$C_{22}H_{30}N_6O_4S$	474	ESI^+	50	35	475	100, 58, 283, 311
180	Stanozolol	$C_{21}H_{32}N_2O$	328	ESI^+	75	37	329	81, 95, 107, 135
181	Strychnine	$C_{21}H_{22}N_2O_2$	334	ESI^+	70	38	335	184, 156, 144, 264, 222
182	Sulfadiazine	$C_{10}H_{10}N_4O_2S$	250	ESI^+	30	13	251	156, 92, 94, 96
183	Sulfadimethoxine	$C_{12}H_{14}N_4O_4S$	310	ESI^+	40	17	311	156, 245, 218, 108, 92
184	Sulfamerazine	$C_{11}H_{12}N_4O_2S$	264	ESI^+	30	15	265	156, 172, 110, 92
185	Sulfamethazine	$C_{12}H_{14}N_4O_2S$	278	ESI^+	35	15	279	186, 156, 124, 92
186	Sulfamethizole	$C_9H_{10}N_4O_2S_2$	270	ESI^+	35	14	271	156, 108, 92
187	Sulfamethoxazole	$C_{10}H_{11}N_3O_3S$	253	ESI^+	25	16	254	156, 188, 147, 108, 92
188	Sulfamethoxypyridazine	$C_{11}H_{12}N_4O_3S$	280	ESI^+	35	15	281	156, 126, 108, 92, 188
189	Sulfanilamide	$C_6H_8O_2N_2S$	172	ESI^+	10	10	173	92,108,156
190	Sulfathiazole	$C_9H_9N_3O_2S_2$	255	ESI^+	40	15	256	156, 108, 92
191	Sulfinpyrazone	$C_{23}H_{20}N_2O_3S$	404	ESI^+	35	19	405	279, 185, 387, 253, 93, 294
192	Sulfisoxazole	$C_{11}H_{13}N_3O_3S$	267	ESI^+	25	11	268	156, 113, 108, 92
193	Sulindac	$C_{20}H_{17}FO_3S$	356	ESI^+	36	25	357	233, 248, 295, 340
194	Synephrine	$C_9H_{13}NO_2$	167	ESI^+	25	7	168	150
195	Tadalafil	$C_{22}H_{19}N_3O_4$	389	ESI^+	30	20	390	268, 135
196	Terbinafine	$C_{21}H_{25}N$	291	ESI^+	25	13	292	141, 170, 93
197	Terfenadine	$C_{32}H_{41}NO_2$	471	ESI^+	40	23	472	436, 454, 58
198	Testosterone	$C_{19}H_{28}O_2$	288	ESI^+	10	15	289	97, 109, 122
199	Tetracaine	$C_{15}H_{24}N_2O_2$	264	ESI^+	25	17	265	220, 176, 72
200	Theobromine	$C_7H_8N_4O_2$	180	ESI^+	25	20	181	138, 67, 163, 110, 122
201	Theophylline	$C_7H_8N_4O_2$	180	ESI^+	40	25	181	96, 69, 124
202	Thiodimethylsildenafil	$C_{23}H_{32}N_6O_3S_2$	504	ESI^+	50	30	505	99, 113, 327, 299, 71, 393

Published, Nov 23, 2012
Revised, Feb 17, 2014
Revised, March 5, 2020
TFDAO0015.02

NO.	Compound	Molecular formula	Molecular weight	Ionization mode	Cone voltage (V)	Collision energy (eV)	Precursor ion (*m/z*)	Product ion (*m/z*)
203	Thiohomosildenafil	$C_{23}H_{32}N_6O_3S_2$	504	ESI^+	60	40	505	113, 99, 73, 299, 327
204	Thioridazine	$C_{21}H_{26}N_2S_2$	370	ESI^+	40	25	371	126, 98
205	Thiosildenafil	$C_{22}H_{30}N_6O_3S_2$	490	ESI^+	50	37	491	341, 100, 58
206	Tinidazole	$C_8H_{13}N_3O_4S$	247	ESI^+	20	10	248	121, 93, 128, 110
207	Tolbutamide	$C_{12}H_{18}N_2O_3S$	270	ESI^-	30	20	269	170
208	Triamcinolone	$C_{21}H_{27}FO_6$	394	ESI^-	33	12	393	363, 345, 325
209	Vardenafil	$C_{23}H_{32}N_6O_4S$	488	ESI^+	50	40	489	151, 114, 99, 72, 58
210	Desulfovardenafil (Vardenafil analogue, 【2-(2-ethoxy-phenyl)-5-methyl-7-propyl-3H-imidazo(51-f)-(1,2,4)triazin-4-one】)	$C_{17}H_{20}N_4O_2$	312	ESI^+	50	31	313	151
211	Xanthinol Niacinate	$C_{13}H_{21}N_5O_4$	311	ESI^+	30	3	312	124
212	Yohimbine	$C_{21}H_{26}N_2O_3$	354	ESI^+	50	30	355	212, 144
213	Zolpidem	$C_{19}H_{21}N_3O$	307	ESI^+	45	25	308	235, 263
214	Cetilistat	$C_{25}H_{39}NO_3$	401	—	—	—	—	—
215	Avanafil	$C_{23}H_{26}ClN_7O_3$	483	ESI^+	30	20	484	375, 155
216	Benproperine	$C_{21}H_{27}NO$	309	ESI^+	40	25	310	126, 91, 84
217	Celecoxib	$C_{17}H_{14}F_3N_3O_2S$	381	ESI^+	40	30	382	362, 382, 300
218	Clozapine	$C_{18}H_{19}ClN_4$	326	ESI^+	25	20	327	270, 84
219	Cyproheptadine	$C_{21}H_{21}N$	287	ESI^+	40	25	288	96, 191
220	Desacetyl bisacodyl	$C_{18}H_{15}NO_2$	277	ESI^+	30	10	278	184
221	2-Diphenylmethylpyrrolidine (Desoxy-D2PM)	$C_{17}H_{19}N$	237	ESI^+	25	17	238	91, 117, 143

Published, Nov 23, 2012
Revised, Feb 17, 2014
Revised, March 5, 2020
TFDAO0015.02

NO.	Compound	Molecular formula	Molecular weight	Ionization mode	Cone voltage (V)	Collision energy (eV)	Precursor ion (*m/z*)	Product ion (*m/z*)
222	Famotidine	$C_8H_{15}N_7O_2S_3$	337	ESI^+	10	12	338	189, 259
223	Hydroxyzine	$C_{21}H_{27}ClN_2O_2$	374	ESI^+	25	13	375	201, 173
224	Lorcaserin	$C_{11}H_{14}ClN$	195	ESI^+	20	25	196	129, 144, 103, 139, 125
225	Nefopam	$C_{17}H_{19}NO$	253	ESI^+	30	20	254	181, 166
226	Norgestrel	$C_{21}H_{28}O_2$	312	ESI^+	40	22	313	109, 107, 135, 245
227	Omeprazole	$C_{17}H_{19}N_3O_3S$	345	ESI^+	25	5	346	198, 168, 149
228	Prilocaine	$C_{13}H_{20}N_2O$	220	ESI^+	30	10	221	86
229	Promethazine	$C_{17}H_{20}N_2S$	284	ESI^+	25	13	285	86, 198, 240
230	Spironolactone	$C_{24}H_{32}O_4S$	416	ESI^+	20	10	417	341, 187
231	Topiramate	$C_{12}H_{21}NO_8S$	339	ESI^-	30	26	338	78, 96
232	Trimethoprim	$C_{14}H_{18}N_4O_3$	290	ESI^+	35	26	291	123, 230, 261, 110

Note: 1. Capillary voltage is 3 kV for each analyte.

2.“ — ” represents that compound cannot be detected by LC-MS/MS.

3. All the parameters can be adjusted depending on the instruments used if the above conditions are not applicable.